

g nodes :  
 8 9 10 11 12 13 22 23 24 25 26 27  
 g/chain nodes :  
 1 2 3 4 5 6 7 14 15 16 17 18 19 20 21 28 29 30 31 32 33 34 35 36 37  
 g/chain bonds :  
 1-2 1-5 1-6 2-3 3-4 4-7 7-8 9-14 10-17 13-35 14-15 15-16 17-18 18-19 19-20  
 20-21 21-22 23-28 24-31 25-32 28-29 29-30 32-33 32-34 35-36 35-37  
 g bonds :  
 8-9 8-13 9-10 10-11 11-12 12-13 22-23 22-27 23-24 24-25 25-26 26-27  
 ct/norm bonds :  
 1-2 2-3 3-4 9-14 13-35 14-15 15-16 18-19 19-20 23-28 25-32 28-29 29-30 32-34  
 35-37  
 ct bonds :  
 1-5 1-6 4-7 7-8 10-17 17-18 20-21 21-22 24-31 32-33 35-36  
 malized bonds :  
 8-9 8-13 9-10 10-11 11-12 12-13 22-23 22-27 23-24 24-25 25-26 26-27

ch level :  
 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS  
 20:CLASS 21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS  
 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS

his

(FILE 'HOME' ENTERED AT 09:13:47 ON 12 AUG 2004)

FILE 'CAPLUS' ENTERED AT 09:13:59 ON 12 AUG 2004  
STRUCTURE UPLOADED  
S L1

FILE 'REGISTRY' ENTERED AT 09:14:50 ON 12 AUG 2004  
11 S L1 FULL

FILE 'CAPLUS' ENTERED AT 09:14:54 ON 12 AUG 2004  
3 S L2 FULL  
0 S L3 AND POLYMORPHIC?  
0 S L3 AND POLYMORPH?

strictly prohibited.

E COVERS 1907 - 12 Aug 2004 VOL 141 ISS 7  
E LAST UPDATED: 11 Aug 2004 (20040811/ED)

This file contains CAS Registry Numbers for easy and accurate  
substance identification.

Loading C:\STNEXP4\QUERIES\861.str

STRUCTURE UPLOADED

d11  
HAS NO ANSWERS  
STR

STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

s11 full  
**REGISTRY INITIATED**  
Structure data SEARCH and crossover from CAS REGISTRY in progress...  
DISPLAY HITSTR (or PHITSTR) to directly view retrieved structures.

SEARCH INITIATED 09:14:50 FILE 'REGISTRY'  
SCREEN SEARCH COMPLETED - 355524 TO ITERATE

100% PROCESSED 355524 ITERATIONS 11 ANSWERS  
SEARCH TIME: 00.00.04

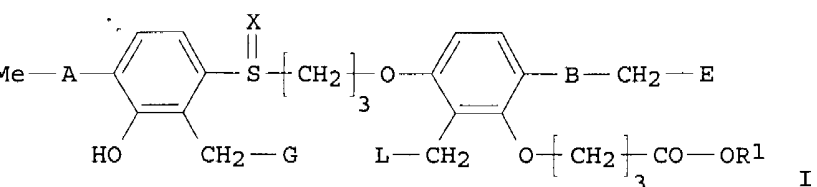
11 SEA SSS FUL L1

3 L2

d 1-3 ibib abs hitstr

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
SESSION NUMBER: 1995:39068 CAPLUS  
DOCUMENT NUMBER: 123:169347  
TITLE: preparation of phenylthiopropoxyphenyloxybutyric acid  
derivatives as leukotriene antagonists  
AUTHOR(S): Ohashi, Mitsuo; Hori, Wataru  
PATENT ASSIGNEE(S): Kyorin Seiyaku Kk, Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
UNIQUELY ACC. NUM. COUNT: 1  
ADDITIONAL INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 06100526	A2	19940412	JP 1992-273717	19920917
PRIORITY APPLN. INFO.:			JP 1992-273717	19920917
OTHER SOURCE(S):	MARPAT	123:169347		



AB Title derivs. I (A, B = CO, hydroxymethylene; E = H, OH, acetoxy; G, L = Et, acetyl, 1-hydroxyethyl, 2-hydroxyethyl, hydroxycarbonylmethyl, lower alkoxy carbonylmethyl; X = void, O, O<sub>2</sub>; R<sup>1</sup> = H, lower alkyl; X = O, O<sub>2</sub> and B = hydroxymethylene when A = carbonyl, E = H, and G = L = Et) or their alkali salts, acting as strong antagonists for leukotrienes C<sub>4</sub>, D<sub>4</sub>, and E<sub>4</sub> and useful for antiasthmatics, are prepared Thus, treating 2'-hydroxy-3'-(2-hydroxypropyl)-4'-mercaptoacetophenone (prepared in 6 steps from 3-allyl-2,4-dihydroxyacetophenone) with Et 4-[6-acetyl-3-(3-bromopropoxy)-2-propylphenoxy]butyrate gave I (A = B = CO, E = H, G = 1-hydroxyethyl, L = Et, R<sup>1</sup> = Et, X = void).

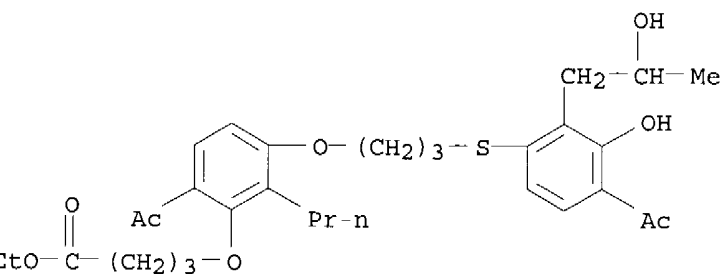
IT 167211-60-1P 167211-72-5P 167211-78-1P  
167211-82-7P 167211-90-7P 167211-91-8P  
167211-92-9P 167211-93-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of phenylthiopropoxyphenyloxybutyric acid derivs. as leukotriene antagonists)

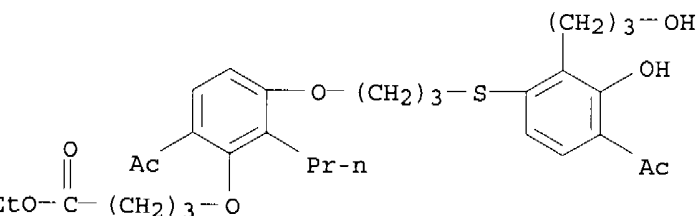
RN 167211-60-1 CAPLUS

CN Butanoic acid, 4-[6-acetyl-3-[3-[[4-acetyl-3-hydroxy-2-(2-hydroxypropyl)phenyl]thio]propoxy]-2-propylphenoxy]-, ethyl ester (9CI)  
(CA INDEX NAME)



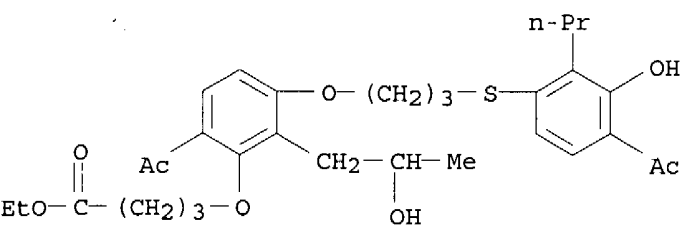
RN 167211-72-5 CAPLUS

CN Butanoic acid, 4-[6-acetyl-3-[3-[[4-acetyl-3-hydroxy-2-(3-hydroxypropyl)phenyl]thio]propoxy]-2-propylphenoxy]-, ethyl ester (9CI)  
(CA INDEX NAME)

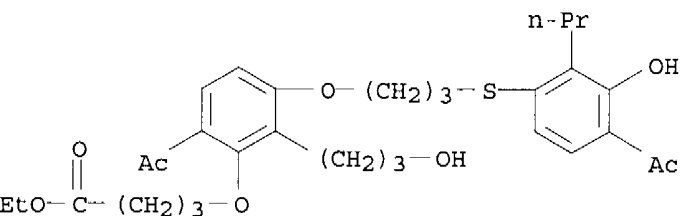


RN 167211-78-1 CAPLUS

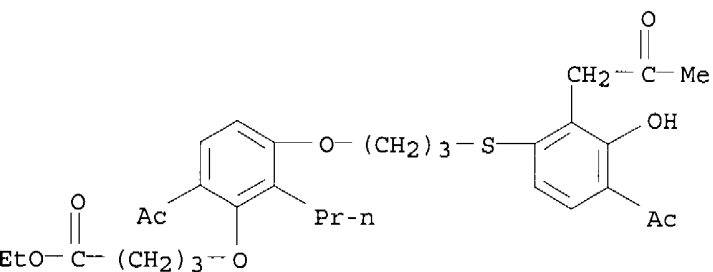
CN Butanoic acid, 4-[6-acetyl-3-[3-[[4-acetyl-3-hydroxy-2-propylphenyl]thio]propoxy]-2-(2-hydroxypropyl)phenoxy]-, ethyl ester (9CI)  
(CA INDEX NAME)



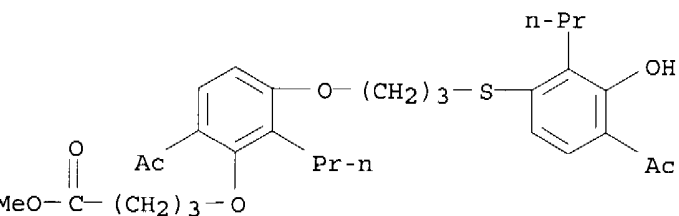
RN 167211-82-7 CAPLUS  
 CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-2-(3-hydroxypropyl)phenoxy]-, ethyl ester (9CI)  
 (CA INDEX NAME)



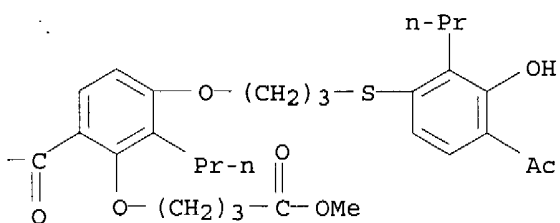
RN 167211-90-7 CAPLUS  
 CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-(2-oxopropyl)phenyl)thio]propoxy]-2-propylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)



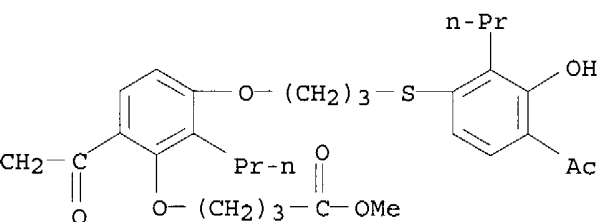
RN 167211-91-8 CAPLUS  
 CN Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-2-propylphenoxy]-, methyl ester (9CI) (CA INDEX NAME)



RN 167211-92-9 CAPLUS  
 CN Butanoic acid, 4-[3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-6-(chloroacetyl)-2-propylphenoxy]-, methyl ester (9CI) (CA INDEX NAME)

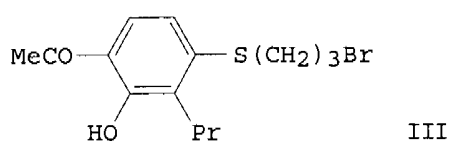
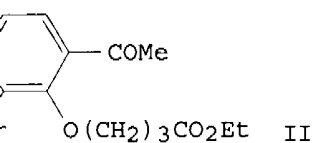
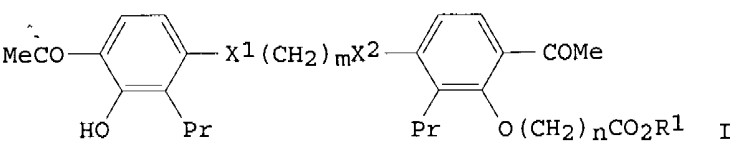


167211-93-0 CAPLUS  
 Butanoic acid, 4-[3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-6-[(acetyloxy)acetyl]-2-propylphenoxy]-, methyl ester (9CI) (CA INDEX NAME)



ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
 SION NUMBER: 1990:138760 CAPLUS  
 IENT NUMBER: 112:138760  
 C: Preparation of phenoxyalkylcarboxylic acid derivatives  
 as antiallergic agents  
 TOR(S): Ohashi, Mitsuo; Awano, Katsuya; Tanaka, Toshio;  
 Kimura, Tetsuya  
 T ASSIGNEE(S): Kyorin Pharmaceutical Co., Ltd., Japan  
 E: Eur. Pat. Appl., 32 pp.  
 CODEN: EPXXDW  
 IENT TYPE: Patent  
 IAGE: English  
 Y ACC. NUM. COUNT: 1  
 IT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 332109	A1	19890913	EP 1989-103897	19890306
EP 332109	B1	19911204		
R: BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
JP 02001459	A2	19900105	JP 1989-38912	19890218
JP 07116125	B4	19951213		
<del>US 4985585</del>	A	19910115	US 1989-313900	19890223
AU 8930884	A1	19890907	AU 1989-30884	19890301
AU 617439	B2	19911128		
CA 1331763	A1	19940830	CA 1989-592555	19890302
HU 50112	A2	19891228	HU 1989-1039	19890303
HU 204030	B	19911128		
HU 208418	B	19931028	HU 1991-2410	19890303
HU 208524	B	19931129	HU 1991-2411	19890303
ES 2045219	T3	19940116	ES 1989-103897	19890306
CN 1036560	A	19891025	CN 1989-101301	19890307
CN 1022407	B	19931013		
ITY APPLN. INFO.:			JP 1988-53374	19880307
			HU 1989-1039	19890303
SOURCE(S):	MARPAT 112:138760			



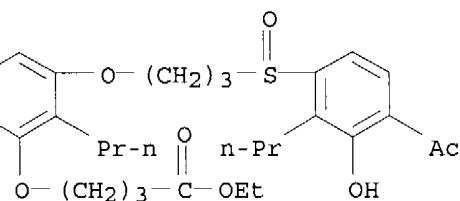
The title compds. (I; R<sup>1</sup> = H, Me, Et; X<sup>1</sup>, X<sup>2</sup> = O, S, SO, SO<sub>2</sub>; X<sup>1</sup> = X<sup>2</sup> ≠ O; m = 2-5; n = 3-8), useful as antiallergic agents, are prepared. A mixture of phenoxybutyrate II, bromopropyl thioether III, KI, and K<sub>2</sub>CO<sub>3</sub> in Me<sub>2</sub>CO was refluxed to give 72.4% I (R<sup>1</sup> = Et, X<sup>1</sup> = S, X<sup>2</sup> = O, m = n = 3). I showed 66.7-96.2% inhibition of leukotriene D<sub>4</sub>-induced bronchoconstriction at 50 mg/kg p.o. in guinea pigs. Addnl. 70 I were also prepared.

125961-80-0P 125961-81-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as antiallergic agent)

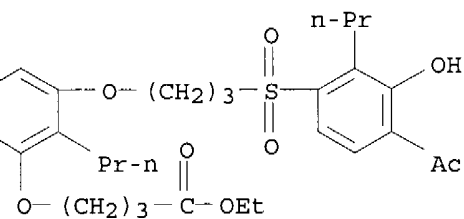
125961-80-0 CAPLUS

Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)sulfinyl]propoxy]-2-propylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)



125961-81-1 CAPLUS

Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)sulfonyl]propoxy]-2-propylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)



ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

SION NUMBER: 1983:575604 CAPLUS

ENT NUMBER: 99:175604

: Anti-SRS-A carboxylic acid derivatives and pharmaceutical formulations containing them

TOR(S): Bantick, John Raymond

T ASSIGNEE(S): Fisons Ltd., UK

E: Eur. Pat. Appl., 67 pp.

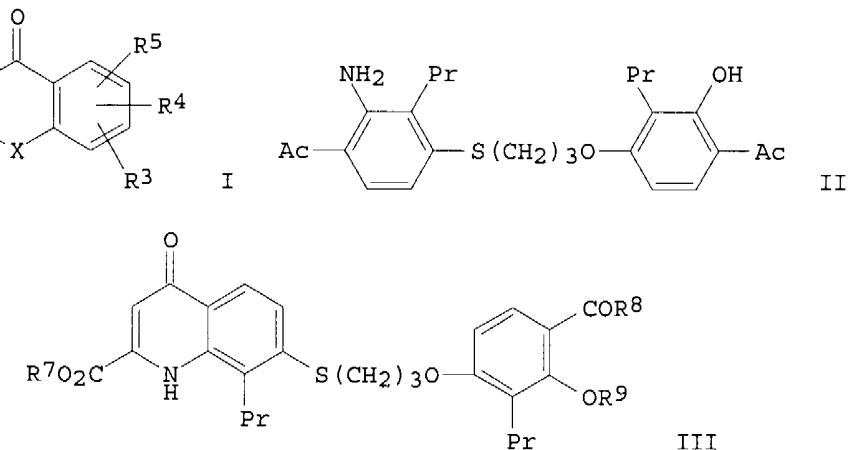
CODEN: EPXXDW

ENT TYPE: Patent

AGE: English

Y ACC. NUM. COUNT: 1  
T INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 79637	A1	19830525	EP 1982-201368	19821101
EP 79637	B1	19870128		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4474788	A	19841002	US 1982-438163	19821101
AT 25251	E	19870215	AT 1982-201368	19821101
JP 58090557	A2	19830530	JP 1982-196883	19821111
ITY APPLN. INFO.:			GB 1981-34186	19811112
			EP 1982-201368	19821101



Anti-allergy (no data) bicyclic compds. I [R, R1 = H, alkyl; RR1 = bond; R2 = CO2H, carboxyalkyl; R3 = substituted OH, SH, NH2; R4, R5 = H, halogen, (un)substituted OH, NH2, alkyl, acyl; X = S, O, NR6 (R6 = H, alkyl)] were prepared. Thus, 3,2,4-Pr(HO)2C6H2Ac reacted with 4,2,3-AcPr(H2N)C6H2S(CH2)3Br to give phenol II, which cyclized with EtO2CCO2Et to give quinoline III [R7 = Et, R8R9 = CH:C(CO2Et)]. The latter compound gave III (R7 = H, R8 = Me, R9 = H) on hydrolysis.

87472-34-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and hydrolysis of)

87472-34-2 CAPLUS

4H-1-Benzopyran-2-propanoic acid, 7-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thiol]propoxy]-4-oxo-8-propyl-, ethyl ester (9CI) (CA INDEX NAME)

